



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 05:50 pm GMT

PDB ID : 1DDM
Title : SOLUTION STRUCTURE OF THE NUMB PTB DOMAIN COMPLEXED
TO A NAK PEPTIDE
Authors : Zwahlen, C.; Li, S.C.; Kay, L.E.; Pawson, T.; Forman-Kay, J.D.
Deposited on : 1999-11-11

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

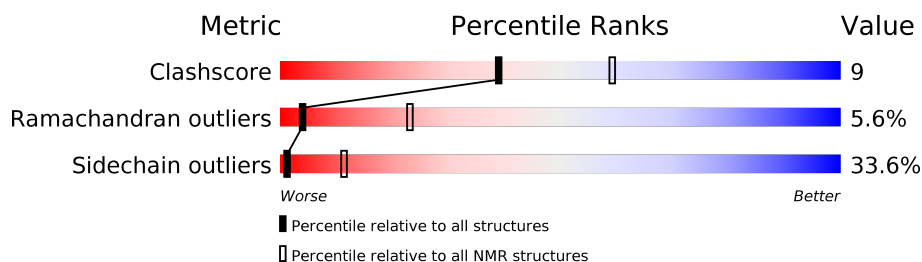
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	135	
2	B	11	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:71-A:153, A:158-A:199, B:2-B:11 (135)	0.48	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 6, 7, 8, 9, 10, 11, 13, 15, 19
2	18, 20
3	5, 12
Single-model clusters	14; 16; 17

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2268 atoms, of which 1114 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NUMB PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	135	Total	C	H	N	O	S	0
			2104	654	1040	203	196	11	

- Molecule 2 is a protein called NUMB ASSOCIATE KINASE.

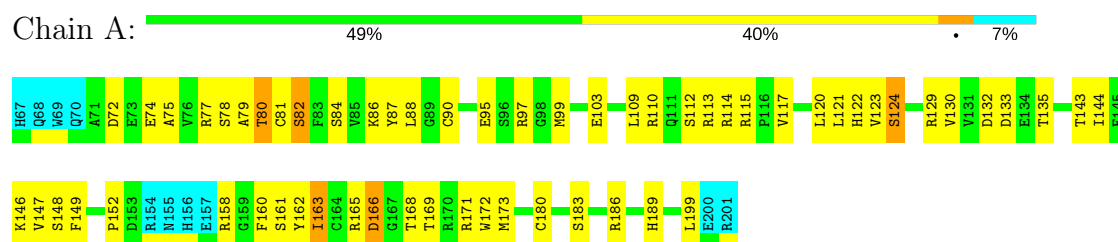
Mol	Chain	Residues	Atoms						Trace
2	B	11	Total	C	H	N	O	S	0
			164	58	74	12	19	1	

4 Residue-property plots [i](#)

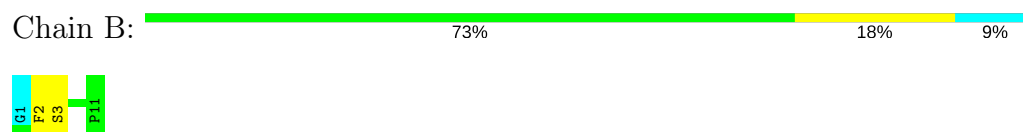
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: NUMB PROTEIN



• Molecule 2: NUMB ASSOCIATE KINASE

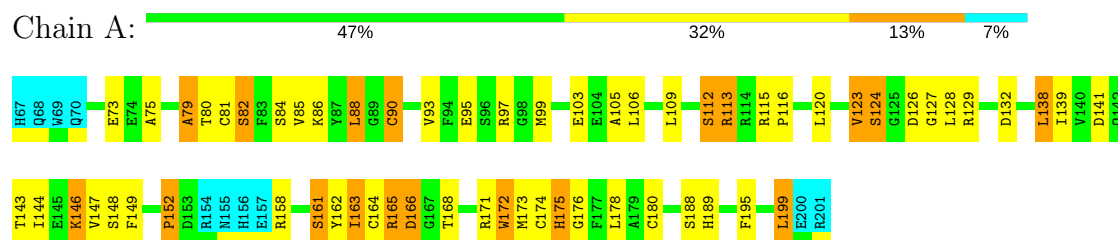


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: NUMB PROTEIN

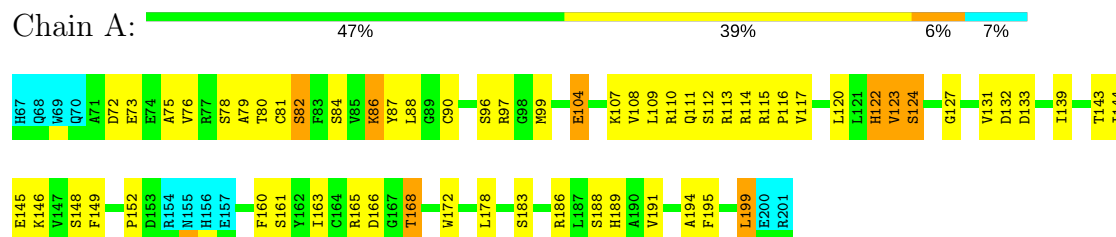


• Molecule 2: NUMB ASSOCIATE KINASE

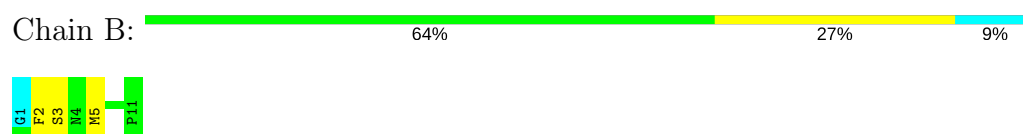


4.2.2 Score per residue for model 2

- Molecule 1: NUMB PROTEIN

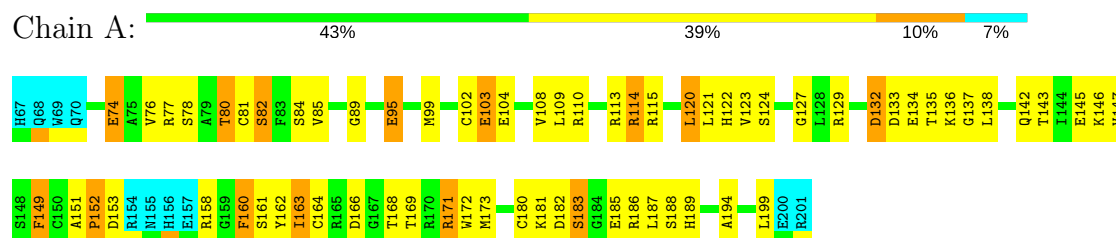


- Molecule 2: NUMB ASSOCIATE KINASE

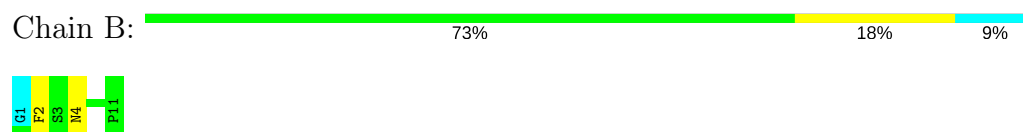


4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: NUMB PROTEIN

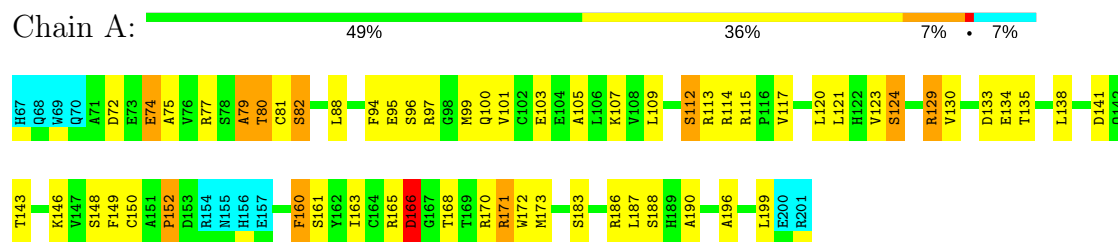


- Molecule 2: NUMB ASSOCIATE KINASE



4.2.4 Score per residue for model 4

- Molecule 1: NUMB PROTEIN

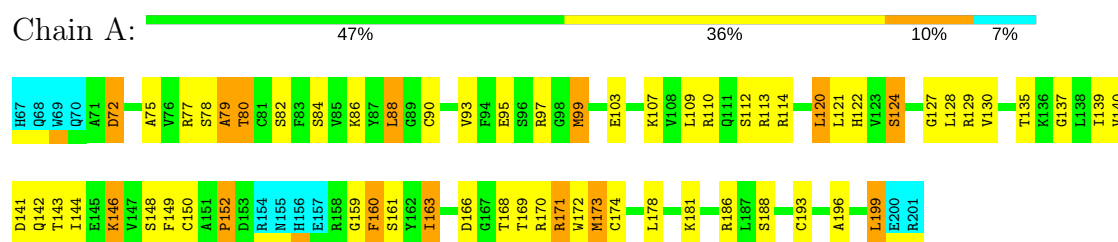


- Molecule 2: NUMB ASSOCIATE KINASE



4.2.5 Score per residue for model 5

- Molecule 1: NUMB PROTEIN

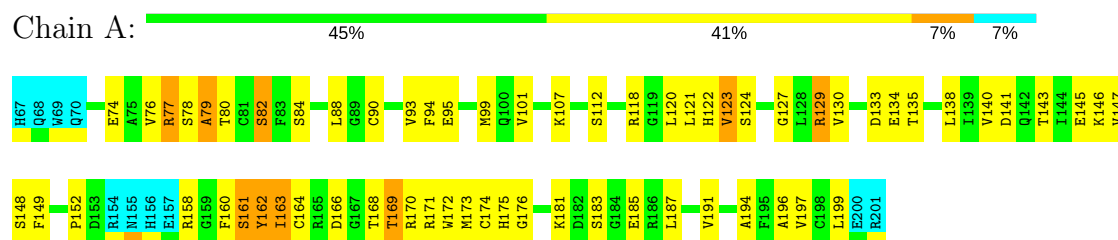


- Molecule 2: NUMB ASSOCIATE KINASE



4.2.6 Score per residue for model 6

- Molecule 1: NUMB PROTEIN



- Molecule 2: NUMB ASSOCIATE KINASE

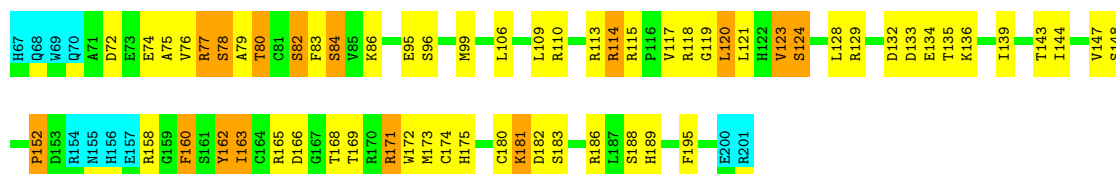




4.2.7 Score per residue for model 7

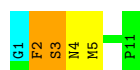
- Molecule 1: NUMB PROTEIN

Chain A: 47% 35% 11% 7%



- Molecule 2: NUMB ASSOCIATE KINASE

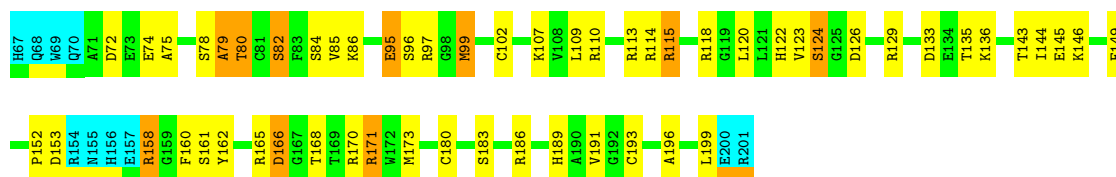
Chain B: 55% 18% 18% 9%



4.2.8 Score per residue for model 8

- Molecule 1: NUMB PROTEIN

Chain A: 51% 34% 7% 7%



- Molecule 2: NUMB ASSOCIATE KINASE

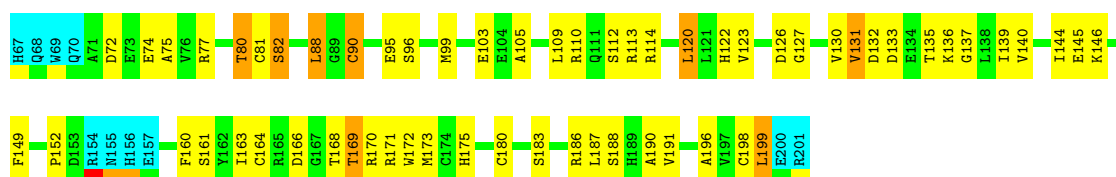
Chain B: 64% 27% 9%



4.2.9 Score per residue for model 9

- Molecule 1: NUMB PROTEIN

Chain A: 48% 39% 6% 7%



- Molecule 2: NUMB ASSOCIATE KINASE

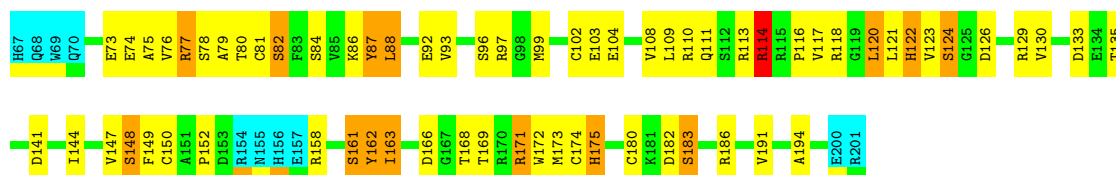
Chain B: 73% 18% 9%



4.2.10 Score per residue for model 10

- Molecule 1: NUMB PROTEIN

Chain A: 44% 38% 10% • 7%



- Molecule 2: NUMB ASSOCIATE KINASE

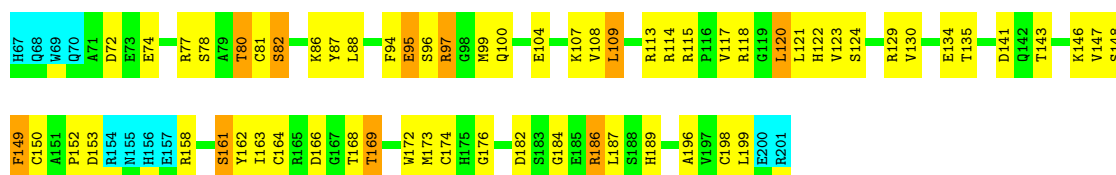
Chain B: 82% 9% 9%



4.2.11 Score per residue for model 11

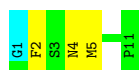
- Molecule 1: NUMB PROTEIN

Chain A: 46% 39% 7% 7%



- Molecule 2: NUMB ASSOCIATE KINASE

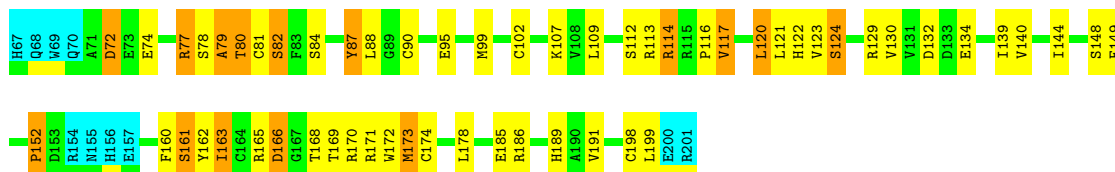
Chain B: 64% 27% 9%



4.2.12 Score per residue for model 12

- Molecule 1: NUMB PROTEIN

Chain A: 50% 31% 11% 7%



- Molecule 2: NUMB ASSOCIATE KINASE

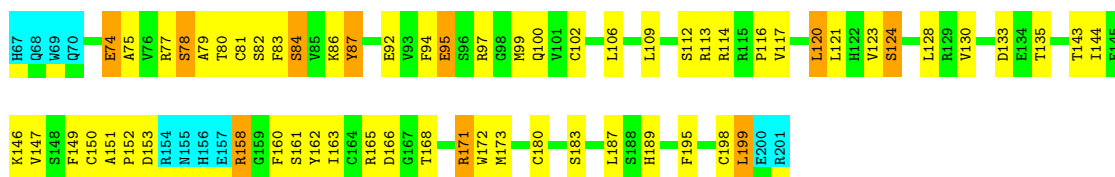
Chain B: 73% 18% 9%



4.2.13 Score per residue for model 13

- Molecule 1: NUMB PROTEIN

Chain A: 47% 38% 7% 7%



- Molecule 2: NUMB ASSOCIATE KINASE

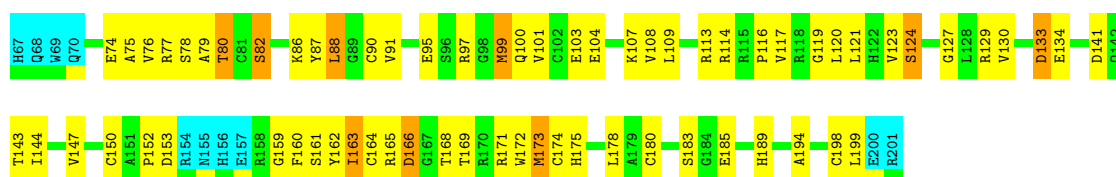
Chain B: 55% 36% 9%



4.2.14 Score per residue for model 14

- Molecule 1: NUMB PROTEIN

Chain A: 43% 43% 7% 7%



- Molecule 2: NUMB ASSOCIATE KINASE

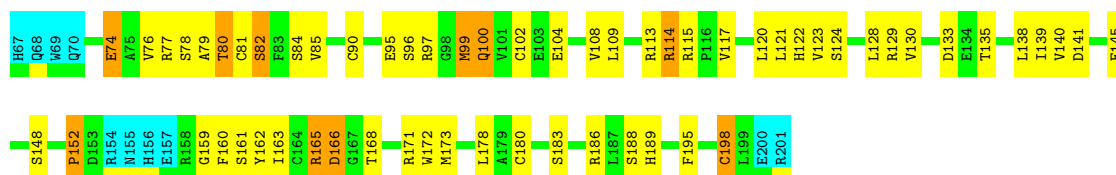
Chain B: 36% 45% 9% 9%



4.2.15 Score per residue for model 15

- Molecule 1: NUMB PROTEIN

Chain A: 48% 37% 7% 7%



- Molecule 2: NUMB ASSOCIATE KINASE

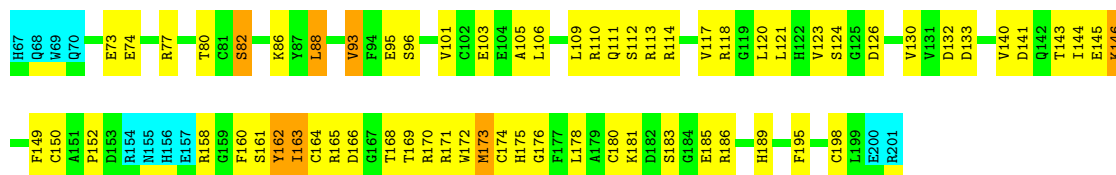
Chain B: 73% 9% 9% 9%



4.2.16 Score per residue for model 16

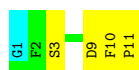
- Molecule 1: NUMB PROTEIN

Chain A: 44% 43% 5% 7%



- Molecule 2: NUMB ASSOCIATE KINASE

Chain B: 55% 36% 9%



4.2.17 Score per residue for model 17

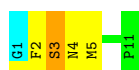
- Molecule 1: NUMB PROTEIN

Chain A: 49% 33% 10% 7%



- Molecule 2: NUMB ASSOCIATE KINASE

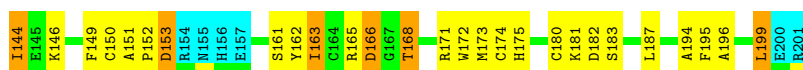
Chain B: 55% 27% 9% 9%



4.2.18 Score per residue for model 18

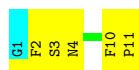
- Molecule 1: NUMB PROTEIN

Chain A: 44% 39% 10% 7%



- Molecule 2: NUMB ASSOCIATE KINASE

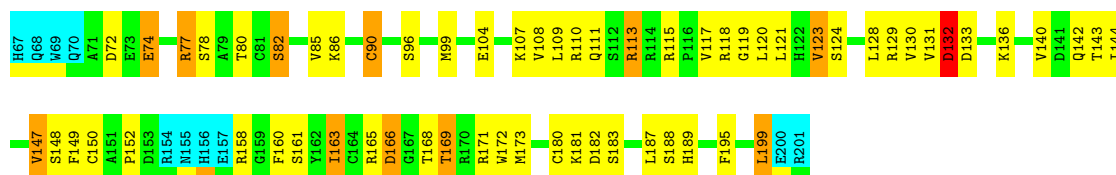
Chain B: 45% 45% 9%



4.2.19 Score per residue for model 19

- Molecule 1: NUMB PROTEIN

Chain A: 47% 37% 8% 7%



• Molecule 2: NUMB ASSOCIATE KINASE

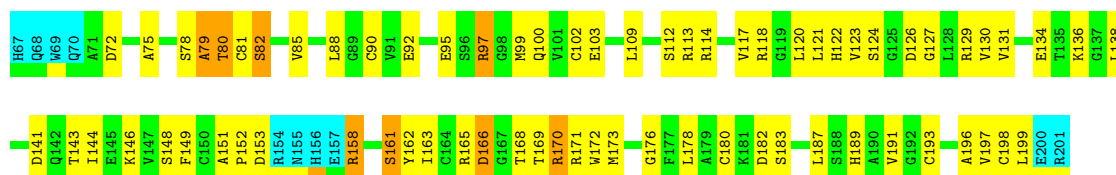
Chain B: 73% 18% 9%



4.2.20 Score per residue for model 20

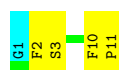
• Molecule 1: NUMB PROTEIN

Chain A: 41% 46% 6% 7%



• Molecule 2: NUMB ASSOCIATE KINASE

Chain B: 55% 36% 9%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS USING ARIA PROTOCOLS FOR AMBIGUOUS RESTRAINTS*.

Of the 150 calculated structures, 20 were deposited, based on the following criterion: *STRUCTURES WITH THE LEAST RESTRAINT VIOLATIONS, STRUCTURES WITH THE LOWEST ENERGY*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	refinement	0.3
CNS	structure solution	0.3

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	964	956	956	18±3
2	B	86	69	69	1±1
All	All	21000	20500	20500	375

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:LEU:HD13	1:A:130:VAL:HG22	0.79	1.55	16	13
1:A:143:THR:HB	1:A:146:LYS:HB2	0.74	1.59	20	10
1:A:169:THR:HG21	1:A:173:MET:HG3	0.71	1.61	5	3
1:A:152:PRO:HD3	2:B:2:PHE:HB2	0.71	1.62	15	4
1:A:81:CYS:HB3	1:A:123:VAL:HB	0.71	1.62	11	10
1:A:196:ALA:HA	1:A:199:LEU:HD12	0.69	1.64	11	6
1:A:76:VAL:HG11	1:A:194:ALA:HA	0.69	1.63	6	6
1:A:169:THR:HG22	1:A:171:ARG:HG3	0.68	1.63	5	4
1:A:163:ILE:HG23	1:A:174:CYS:HB3	0.68	1.66	16	1
1:A:123:VAL:HG11	1:A:191:VAL:HA	0.67	1.65	8	6
1:A:102:CYS:HB3	1:A:161:SER:HB2	0.67	1.67	15	3
1:A:109:LEU:HD23	1:A:114:ARG:HG3	0.66	1.67	14	14
1:A:84:SER:HB2	1:A:181:LYS:HE2	0.66	1.67	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:THR:HA	1:A:122:HIS:HB3	0.64	1.69	3	8
1:A:149:PHE:HB2	1:A:163:ILE:HD12	0.64	1.69	19	2
1:A:74:GLU:HA	1:A:77:ARG:HG3	0.64	1.70	7	12
1:A:79:ALA:HA	1:A:124:SER:HB2	0.62	1.69	1	7
1:A:127:GLY:HA2	1:A:143:THR:HA	0.62	1.72	3	7
1:A:163:ILE:HG23	1:A:174:CYS:HB2	0.62	1.71	1	8
1:A:149:PHE:HB2	2:B:3:SER:HB3	0.61	1.70	5	2
1:A:152:PRO:HA	1:A:160:PHE:HA	0.61	1.72	12	4
1:A:86:LYS:HD2	1:A:116:PRO:HB2	0.61	1.73	2	1
1:A:169:THR:HG21	1:A:173:MET:HB2	0.60	1.73	14	7
1:A:171:ARG:HD2	1:A:173:MET:HG3	0.60	1.74	13	2
1:A:82:SER:HB2	1:A:123:VAL:HG23	0.59	1.74	10	16
1:A:129:ARG:HG2	1:A:138:LEU:HD11	0.59	1.73	3	2
1:A:124:SER:O	1:A:144:ILE:HD11	0.59	1.96	14	10
1:A:158:ARG:HG2	1:A:183:SER:N	0.58	2.13	10	1
1:A:181:LYS:HB2	1:A:186:ARG:HD2	0.56	1.78	17	1
1:A:161:SER:HB3	1:A:176:GLY:HA2	0.56	1.77	1	4
1:A:119:GLY:HA3	1:A:132:ASP:HA	0.55	1.78	18	3
1:A:96:SER:HA	1:A:101:VAL:HG21	0.55	1.79	16	1
1:A:130:VAL:HG23	1:A:140:VAL:HB	0.55	1.79	16	6
1:A:88:LEU:HA	1:A:116:PRO:HA	0.55	1.79	1	2
1:A:105:ALA:O	1:A:109:LEU:HD12	0.54	2.01	16	5
1:A:121:LEU:HD23	1:A:187:LEU:HD23	0.54	1.79	20	5
1:A:158:ARG:HG2	1:A:183:SER:H	0.54	1.62	8	1
1:A:149:PHE:HA	2:B:4:ASN:HB3	0.54	1.77	8	1
1:A:165:ARG:HA	1:A:172:TRP:HA	0.54	1.80	17	2
1:A:149:PHE:HB2	2:B:3:SER:HB2	0.54	1.79	1	2
1:A:166:ASP:HB3	1:A:170:ARG:HA	0.53	1.78	8	4
1:A:196:ALA:HA	1:A:199:LEU:HD11	0.53	1.81	9	3
1:A:120:LEU:HD13	1:A:121:LEU:N	0.52	2.19	10	1
1:A:122:HIS:CE1	1:A:131:VAL:HG23	0.52	2.40	2	1
1:A:149:PHE:HB3	2:B:3:SER:HB2	0.52	1.82	17	1
1:A:121:LEU:HD11	1:A:128:LEU:HD23	0.52	1.82	15	1
1:A:75:ALA:HB1	1:A:80:THR:O	0.52	2.04	5	12
1:A:159:GLY:HA3	1:A:178:LEU:HD23	0.52	1.82	15	2
2:B:10:PHE:HB2	2:B:11:PRO:HD3	0.51	1.83	13	4
1:A:143:THR:O	1:A:147:VAL:HG22	0.51	2.06	11	3
1:A:146:LYS:HE2	1:A:168:THR:HG21	0.51	1.82	17	1
1:A:102:CYS:HB2	1:A:151:ALA:HB3	0.51	1.83	3	1
1:A:122:HIS:HE1	1:A:131:VAL:HG23	0.51	1.66	2	1
1:A:135:THR:HG23	1:A:137:GLY:H	0.51	1.66	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:CYS:SG	1:A:190:ALA:HB1	0.50	2.47	9	2
1:A:90:CYS:N	1:A:109:LEU:HD21	0.50	2.22	19	2
1:A:144:ILE:HD13	1:A:194:ALA:HB1	0.50	1.84	17	1
1:A:186:ARG:HH11	1:A:187:LEU:HB2	0.50	1.66	11	1
1:A:85:VAL:HG12	1:A:187:LEU:HD21	0.49	1.83	18	1
1:A:89:GLY:HA3	1:A:114:ARG:HD3	0.49	1.83	3	1
1:A:82:SER:HB2	1:A:123:VAL:H	0.49	1.67	7	4
1:A:130:VAL:HG12	1:A:139:ILE:HD12	0.49	1.83	9	1
1:A:90:CYS:HB3	1:A:175:HIS:HD2	0.48	1.66	1	1
1:A:83:PHE:HB2	1:A:187:LEU:HD11	0.48	1.85	13	1
1:A:106:LEU:HA	1:A:109:LEU:HD12	0.48	1.83	7	2
1:A:127:GLY:HA2	1:A:144:ILE:HG13	0.48	1.86	9	2
1:A:100:GLN:HB3	1:A:102:CYS:SG	0.47	2.48	17	1
1:A:88:LEU:O	1:A:109:LEU:HD22	0.47	2.09	14	1
1:A:83:PHE:HB3	1:A:181:LYS:HD2	0.47	1.86	7	1
1:A:81:CYS:O	1:A:122:HIS:HA	0.47	2.10	18	5
1:A:88:LEU:O	1:A:114:ARG:HB2	0.47	2.09	10	2
2:B:4:ASN:HD21	2:B:7:PHE:HB3	0.47	1.70	1	1
1:A:88:LEU:HD23	1:A:116:PRO:HB3	0.47	1.86	17	1
1:A:106:LEU:HD11	1:A:178:LEU:HG	0.47	1.87	16	2
1:A:87:TYR:O	1:A:116:PRO:HA	0.46	2.11	18	6
1:A:95:GLU:HG3	1:A:97:ARG:HG3	0.46	1.87	11	1
1:A:104:GLU:O	1:A:108:VAL:HG23	0.46	2.11	14	7
1:A:162:TYR:HE1	1:A:175:HIS:HB2	0.46	1.71	16	1
1:A:103:GLU:HG2	1:A:153:ASP:HA	0.46	1.86	3	1
1:A:120:LEU:HD12	1:A:122:HIS:CE1	0.46	2.46	11	3
1:A:102:CYS:SG	1:A:151:ALA:HB3	0.46	2.51	13	3
1:A:193:CYS:O	1:A:197:VAL:HG23	0.46	2.11	20	1
1:A:138:LEU:HD21	1:A:141:ASP:HB2	0.46	1.86	20	2
1:A:88:LEU:HB3	1:A:109:LEU:HB3	0.45	1.87	12	2
1:A:195:PHE:O	1:A:199:LEU:HG	0.45	2.12	1	5
1:A:93:VAL:HG21	1:A:101:VAL:HG11	0.45	1.87	16	1
1:A:82:SER:CB	1:A:123:VAL:HG23	0.45	2.42	7	11
1:A:95:GLU:O	1:A:97:ARG:HG2	0.45	2.12	20	2
1:A:149:PHE:HA	2:B:4:ASN:ND2	0.45	2.27	5	1
1:A:88:LEU:HB2	1:A:109:LEU:HD22	0.44	1.89	5	1
1:A:120:LEU:HD12	1:A:121:LEU:O	0.44	2.12	7	1
1:A:161:SER:HB3	1:A:175:HIS:O	0.44	2.13	9	1
1:A:162:TYR:CE1	1:A:175:HIS:HB2	0.44	2.47	7	4
1:A:150:CYS:O	2:B:2:PHE:HB3	0.44	2.13	4	1
1:A:84:SER:HA	1:A:120:LEU:HD22	0.44	1.88	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:LEU:HD23	1:A:116:PRO:HG3	0.43	1.88	1	1
1:A:130:VAL:HB	1:A:139:ILE:HG13	0.43	1.90	15	2
1:A:84:SER:HB3	1:A:180:CYS:HB3	0.43	1.88	7	2
1:A:90:CYS:HB3	1:A:175:HIS:ND1	0.43	2.28	9	1
1:A:186:ARG:NH1	1:A:187:LEU:HB2	0.43	2.28	11	1
1:A:138:LEU:HD21	1:A:141:ASP:HB3	0.43	1.91	1	1
1:A:143:THR:HG22	1:A:144:ILE:H	0.43	1.73	17	1
1:A:152:PRO:O	1:A:160:PHE:HA	0.43	2.14	17	1
1:A:119:GLY:HA2	1:A:133:ASP:HB2	0.43	1.91	14	1
1:A:158:ARG:HG2	1:A:182:ASP:HA	0.42	1.91	20	1
1:A:187:LEU:O	1:A:191:VAL:HG23	0.42	2.14	20	1
1:A:143:THR:H	1:A:146:LYS:HB3	0.42	1.74	5	1
1:A:165:ARG:HH21	2:B:10:PHE:HB3	0.42	1.75	15	1
1:A:195:PHE:HB3	2:B:4:ASN:HB2	0.42	1.90	7	1
1:A:195:PHE:HA	1:A:198:CYS:HB2	0.42	1.90	15	1
1:A:181:LYS:CB	1:A:186:ARG:HD2	0.42	2.45	17	1
1:A:143:THR:HG22	1:A:145:GLU:H	0.42	1.75	16	1
1:A:184:GLY:H	1:A:186:ARG:CZ	0.42	2.28	11	1
1:A:97:ARG:HA	1:A:149:PHE:HZ	0.42	1.75	11	1
1:A:166:ASP:HA	1:A:170:ARG:N	0.42	2.30	12	1
1:A:109:LEU:HD23	1:A:114:ARG:CG	0.41	2.45	2	1
1:A:102:CYS:HB3	1:A:161:SER:OG	0.41	2.14	12	1
1:A:132:ASP:O	1:A:136:LYS:HD3	0.41	2.15	3	1
1:A:99:MET:HG3	1:A:100:GLN:N	0.41	2.30	15	1
1:A:161:SER:OG	1:A:176:GLY:HA2	0.41	2.16	16	1
1:A:152:PRO:HA	1:A:160:PHE:HB3	0.41	1.93	5	1
1:A:82:SER:HB3	1:A:121:LEU:O	0.41	2.16	7	1
1:A:140:VAL:HG13	1:A:142:GLN:HG2	0.41	1.91	18	1
1:A:87:TYR:HB3	1:A:117:VAL:HG23	0.41	1.92	12	1
1:A:120:LEU:HD12	1:A:122:HIS:CD2	0.41	2.51	9	2
1:A:88:LEU:HD13	1:A:109:LEU:HB2	0.41	1.92	16	2
1:A:112:SER:O	1:A:113:ARG:HB2	0.41	2.16	4	2
1:A:129:ARG:HA	1:A:140:VAL:O	0.40	2.16	15	1
2:B:7:PHE:HD1	2:B:9:ASP:H	0.40	1.58	14	1
1:A:187:LEU:N	1:A:187:LEU:HD12	0.40	2.31	6	1
1:A:131:VAL:HG12	1:A:136:LYS:HA	0.40	1.93	9	1
1:A:75:ALA:HB3	1:A:81:CYS:SG	0.40	2.57	9	1
1:A:91:VAL:HG13	1:A:109:LEU:CD2	0.40	2.46	14	1
1:A:159:GLY:HA2	1:A:178:LEU:HA	0.40	1.92	5	1
1:A:129:ARG:HD3	1:A:138:LEU:HD11	0.40	1.92	4	1

6.3 Torsion angles

6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	125/135 (93%)	95±3 (76±2%)	23±2 (18±2%)	7±2 (6±2%)	4	22
2	B	9/11 (82%)	7±1 (73±14%)	2±1 (24±13%)	0±0 (3±5%)	8	39
All	All	2680/2920 (92%)	2037 (76%)	493 (18%)	150 (6%)	4	23

All 28 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	168	THR	17
1	A	152	PRO	17
1	A	79	ALA	15
1	A	95	GLU	13
1	A	183	SER	13
1	A	78	SER	11
1	A	166	ASP	11
1	A	123	VAL	6
1	A	87	TYR	5
1	A	182	ASP	5
1	A	165	ARG	4
2	B	3	SER	4
1	A	115	ARG	3
1	A	80	THR	3
1	A	99	MET	3
1	A	113	ARG	2
1	A	188	SER	2
1	A	114	ARG	2
1	A	101	VAL	2
2	B	9	ASP	2
1	A	153	ASP	2
1	A	126	ASP	2
1	A	138	LEU	1
1	A	171	ARG	1
1	A	112	SER	1
1	A	150	CYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	132	ASP	1
1	A	148	SER	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	105/115 (91%)	68±3 (65±3%)	37±3 (35±3%)	1	9
2	B	10/10 (100%)	8±1 (81±10%)	2±1 (19±10%)	5	37
All	All	2300/2500 (92%)	1527 (66%)	773 (34%)	1	11

All 96 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	82	SER	20
1	A	120	LEU	19
1	A	163	ILE	19
1	A	172	TRP	19
2	B	2	PHE	18
1	A	99	MET	18
1	A	171	ARG	17
1	A	113	ARG	16
1	A	166	ASP	16
1	A	124	SER	15
1	A	133	ASP	15
1	A	162	TYR	14
1	A	160	PHE	14
1	A	161	SER	14
1	A	129	ARG	13
1	A	189	HIS	13
1	A	186	ARG	13
1	A	117	VAL	13
1	A	148	SER	13
1	A	173	MET	12
1	A	80	THR	12
1	A	84	SER	12

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Mol	Chain	Res	Type	Models (Total)
1	A	86	LYS	12
1	A	72	ASP	12
1	A	88	LEU	12
1	A	180	CYS	12
1	A	90	CYS	11
1	A	97	ARG	11
1	A	110	ARG	11
1	A	149	PHE	11
1	A	158	ARG	10
1	A	112	SER	10
1	A	199	LEU	10
1	A	107	LYS	9
1	A	132	ASP	9
1	A	103	GLU	9
1	A	96	SER	9
1	A	165	ARG	9
1	A	198	CYS	9
1	A	118	ARG	8
1	A	188	SER	8
2	B	3	SER	8
1	A	135	THR	8
1	A	115	ARG	8
1	A	134	GLU	8
1	A	74	GLU	8
1	A	78	SER	8
1	A	147	VAL	8
1	A	164	CYS	8
1	A	150	CYS	7
1	A	141	ASP	7
1	A	181	LYS	7
1	A	77	ARG	7
1	A	100	GLN	6
2	B	5	MET	6
1	A	73	GLU	6
1	A	85	VAL	6
1	A	114	ARG	6
1	A	145	GLU	6
1	A	146	LYS	5
1	A	93	VAL	5
1	A	170	ARG	5
1	A	185	GLU	5
1	A	169	THR	5

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Mol	Chain	Res	Type	Models (Total)
1	A	168	THR	5
1	A	153	ASP	5
2	B	4	ASN	5
1	A	95	GLU	5
1	A	128	LEU	5
1	A	136	LYS	4
1	A	111	GLN	4
1	A	175	HIS	4
1	A	144	ILE	4
1	A	131	VAL	4
1	A	92	GLU	4
1	A	139	ILE	4
1	A	94	PHE	4
1	A	126	ASP	4
1	A	142	GLN	3
1	A	183	SER	3
1	A	178	LEU	3
1	A	101	VAL	2
1	A	87	TYR	2
1	A	76	VAL	2
1	A	182	ASP	2
1	A	193	CYS	2
1	A	122	HIS	2
1	A	187	LEU	2
1	A	195	PHE	2
1	A	174	CYS	1
1	A	106	LEU	1
2	B	8	GLU	1
1	A	109	LEU	1
1	A	104	GLU	1
1	A	140	VAL	1
1	A	197	VAL	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided